# Exploring models Summary, explainability, and prediction

R.W. Oldford



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They suggested that objectives in data analysis that are comparable to those of experimentation are<sup>1</sup>

- 1. "to achieve more specific description of what is loosely known or suspected;
- "to find unanticipated aspects in the data, and to suggest unthought-of models for the data's summarization and exposure;
- "to employ the data to assess the (always incomplete) adequacy of a contemplated model;
- "to provide both incentives and guidance for further analysis of the data; and
- 5. "to keep the investigator usefully stimulated while he absorbs the feeling of his data and considers what to do next."



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Here, model is generally (though not exclusively) to be understood in a more formal mathematical sense. Tukey and Wilk also cautioned against taking them too seriously. In their words, "Models must be used but must never be believed."

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- we make inferences from the model about  $\mu()$  using the estimator  $\widetilde{\mu}(x_1,\ldots,x_p)$  and its distribution.
- when  $\mu()$  is expressed in terms of a finite number of unknown parameters, say  $\theta_1,\ldots,\theta_k$ , we say that it is a **parametric model** with parameter estimates  $\widehat{\theta}_1,\ldots,\widehat{\theta}_k$  and corresponding estimators  $\widetilde{\theta}_1,\ldots,\widetilde{\theta}_k$ .



## Regression models

$$Y = \mu(x_1, \dots, x_q) + R$$

$$E(R) = 0$$

$$R \sim F_R(r; \sigma)$$

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Such models include the linear model whereby

$$\mu(x_1,\ldots,x_q)=\theta_0+\theta_1x_1+\cdots+\theta_px_p.$$

Here linear refers to the mean model being linear in the unknown parameters  $\theta_i$ . (There are non-linear regression models as well.)



#### Generalizing the linear model

A slight generalization is to instead model a function of the conditional mean, as in the so-called **generalized linear model** where now there is a known function  $g(\mu)$  called the **link** function and we model

$$g(\mu(x_1,\ldots,x_q)) = \theta_0 + \theta_1x_1 + \cdots + \theta_px_p$$

with everything else as before.

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Another way we might generalize the linear model is to model the mean as

$$\mu(x_1,\ldots,x_q)=\theta+h_1(x_1)+\cdots+h_p(x_p)$$

where  $h_i(x_i)$  are arbitrary functions, each of only a single explanatory variate  $(x_i)$ . This is called an **additive model** (being additive in functions of the explanatory variates).



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These are only a few of the many models that are possible.



Providers of response models in R try to have a consistent modelling interface.



<sup>&</sup>lt;sup>2</sup>Formulas in R generalize Wilkinson-Rogers notation developed much earlier for specifying linear and generalized linear models.

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specifies a linear model with y as the response and the variates named x1, x2, and x3 as the explanatory variates (or **predictors**). The variates x1, x2, and x3 are sometimes called the **terms** of the model.

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- the intercept term θ<sub>0</sub> is always implicitly assumed to be part of the model; it can be removed by adding a -1 term to the model.
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  - + b indicates adding a separate term b to the model,
  - b indicates removing the term b from the model,
  - ▶ a:b indicates an interaction term between a and b be added,
  - ▶ a\*b is a short-hand equivalent to a + b + a:b,
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- poly(x, p) specifies a polynomial in x of degree p (uses orthogonal polynomials)



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  - often also produces prediction intervals for a new observation and confidence intervals for the conditional mean



#### Fitted models

- summary(myfit) should return (and print) a statistical summary of the data such as
  - ▶ an overall measure of the quality of the fit
  - ▶ an indication of the statistical significance of each term in the model
- plot(fit) should produce one or more plots that summarize the fit and provide some diagnostic tools for assessing its quality
- predict(fit , ...) provide predictions of the response (typically its estimated conditional mean) at any collection of variate values
  - requires a data set of new values for every variate named in the model formula
  - often also produces prediction intervals for a new observation and confidence intervals for the conditional mean
- ▶ str(fit) reveals the structure of the fitted model. Here we expect to also find myfit\$residuals containing the residuals, or deviations, of the observed responses from their fitted conditional mean

#### Facebook data - fitting linear models

Linear models are fitted in R using the lm() function.

```
fit1 <- lm(log10(Impressions) ~ Paid, data = facebook)
summary(fit1)</pre>
```

```
##
## Call:
## lm(formula = log10(Impressions) ~ Paid, data = facebook)
##
## Residuals:
##
       Min
                 10 Median
                                  30
                                          Max
## -1.25955 -0.32022 -0.09619 0.28444 2.03001
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 4.01543 0.02655 151.236 < 2e-16 ***
## Paid
               0.21142 0.05031 4.203 3.13e-05 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5038 on 497 degrees of freedom
    (1 observation deleted due to missingness)
## Multiple R-squared: 0.03432, Adjusted R-squared: 0.03238
## F-statistic: 17.66 on 1 and 497 DF, p-value: 3.128e-05
```



#### Facebook data - contents of linear fits

# Extracting contents

```
fit1$coefficients
## (Intercept)
                     Paid
##
     4.0154262
                 0.2114186
head(model.matrix(fit1))
     (Intercept) Paid
##
## 1
## 2
## 3
## 4
## 6
head(fit1$residuals)
##
```

```
## 1 2 3 4 5 6

## -0.3086231 0.2646283 -0.3746467 0.7175934 0.1179211 0.3036590

# And prediction (based on the estimated mean don't forget)

predict(fit1, newdata = data.frame(Paid = c(0,1)))
```

```
## 4.015426 4.226845
# The predicted mean increase in Impressions for paid advertising
diff(10^predict(fit1, newdata = data.frame(Paid = c(0,1))))
```

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##

#### Facebook data - linear model with a factor

# Recall that Category took values Product, Inspiration, Action

```
fit2 <- lm(log10(Impressions) \sim Category, data = facebook) summary(fit2)
```

```
##
## Call:
## lm(formula = log10(Impressions) ~ Category, data = facebook)
##
## Residuals:
              1Q Median
##
      Min
                              30
                                    Max
## -1.3727 -0.3074 -0.1079 0.2854 1.9168
##
## Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                     4.12860 0.03482 118.583 <2e-16 ***
## CategoryInspiration -0.09723 0.05379 -1.807 0.0713 .
## CategoryProduct -0.09449 0.05672 -1.666 0.0963 .
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5105 on 497 degrees of freedom
## Multiple R-squared: 0.008645, Adjusted R-squared: 0.004655
## F-statistic: 2.167 on 2 and 497 DF, p-value: 0.1156
```



### Facebook data - contents of linear model with a factor

#### Extracting contents

```
fit2$coefficients
##
           (Intercept) CategoryInspiration
                                               CategoryProduct
##
            4.12860385
                               -0.09722799
                                                   -0.09449137
head(model.matrix(fit2))
##
     (Intercept) CategoryInspiration CategoryProduct
## 1
## 2
## 3
## 6
head(fit2$residuals)
##
## -0.32730938 0.24594205 -0.39059638 0.91032577
                                                    0.09923478 0.28497275
# And prediction on original scale of Impressions
10 predict(fit2, newdata = data.frame(Category = factor(levels(facebook$Category))))
##
```

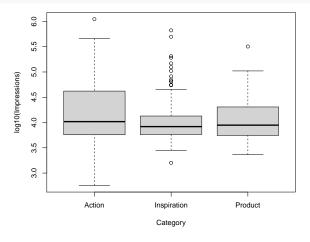
Conclusions?

## 13446.33 10749.19 10817.14



Formulas are also used by other functions (e.g. boxplot())

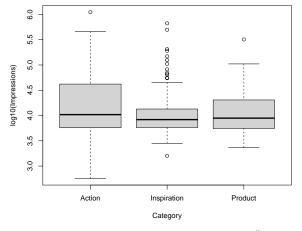
boxplot(log10(Impressions) ~ Category, data = facebook, col = "lightgrey")





Formulas are also used by other functions (e.g. boxplot())

boxplot(log10(Impressions) ~ Category, data = facebook, col = "lightgrey")

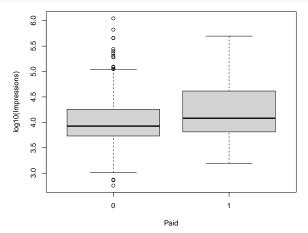


Comments? How is this "model" different from the one constructed by lm()'?



#### How about log10(Impressions) as a function of Paid?

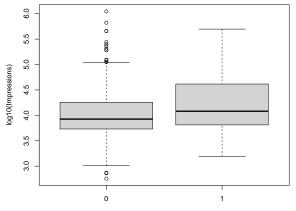
boxplot(log10(Impressions) ~ Paid, data = facebook, col = "lightgrey")





#### How about log10(Impressions) as a function of Paid?

boxplot(log10(Impressions) ~ Paid, data = facebook, col = "lightgrey")

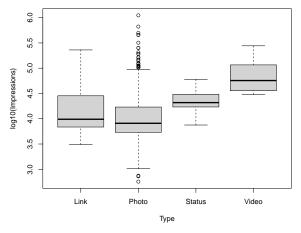


Paid



#### How about log10(Impressions) as a function of Type?

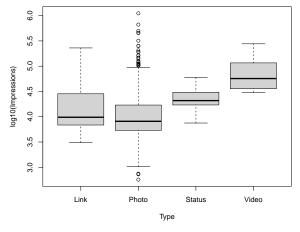
boxplot(log10(Impressions) ~ Type, data = facebook, col = "lightgrey")





#### How about log10(Impressions) as a function of Type?

boxplot(log10(Impressions) ~ Type, data = facebook, col = "lightgrey")

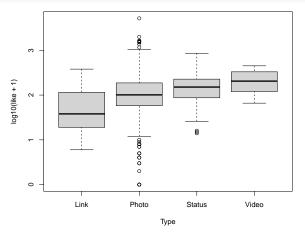






How about log10(Impressions) as a function of Type?

boxplot(log10(like +1) ~ Type, data = facebook, col = "lightgrey")

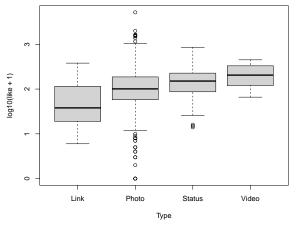






How about log10(Impressions) as a function of Type?

boxplot(log10(like +1) ~ Type, data = facebook, col = "lightgrey")

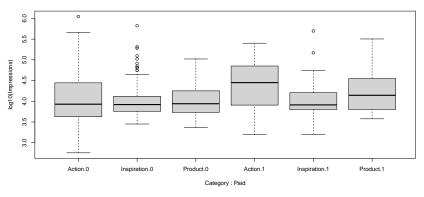


Comments? How is this model formula interpreted?



This works well when explanatory variates are categorical.

boxplot(log10(Impressions) ~ Category + Paid, data = facebook, col = "lightgrey")

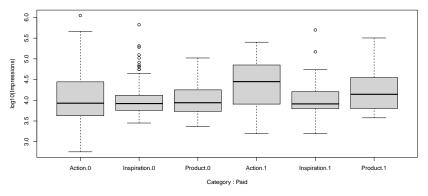


Comments?



This works well when explanatory variates are categorical.

boxplot(log10(Impressions) ~ Category + Paid, data = facebook, col = "lightgrey")



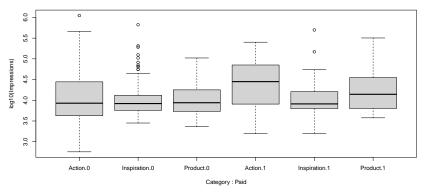
#### Comments?

Note the labels on the horizontal axis.



This works well when explanatory variates are categorical.

```
boxplot(log10(Impressions) ~ Category + Paid, data = facebook, col = "lightgrey")
```



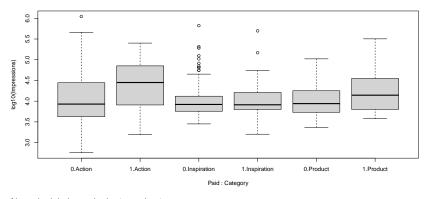
#### Comments?

Note the labels on the horizontal axis. How is this model formula interpreted?



### What has changed here?

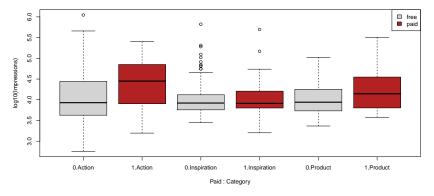
boxplot(log10(Impressions) ~ Paid + Category, data = facebook, col = "lightgrey")



Note the labels on the horizontal axis.



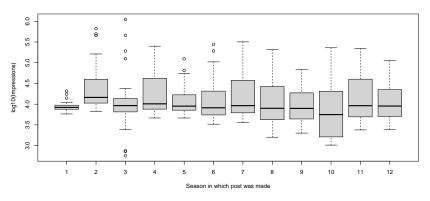
### What has changed here?



Note the labels on the horizontal axis.

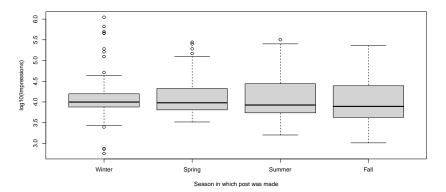


### By month

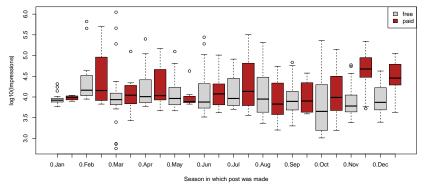




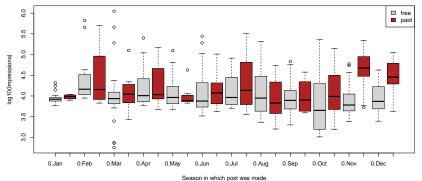
### A numeric variate could be made categorical using cut()



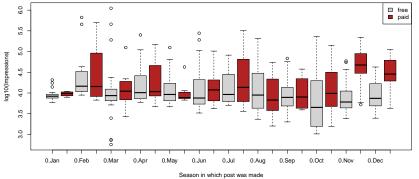




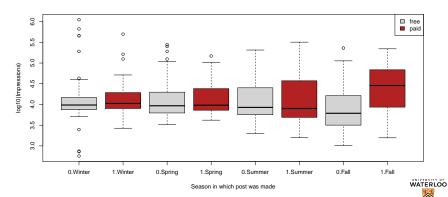


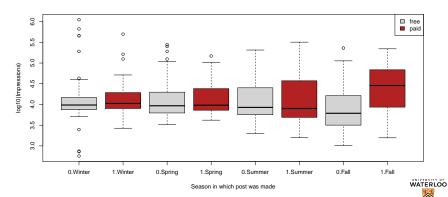




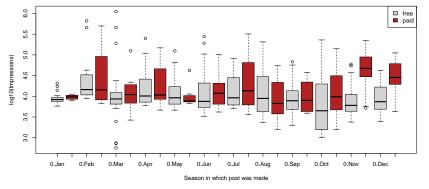






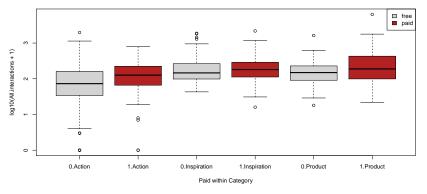


### Or how about?





### Change response.





### Change response. Fitted model

```
fit3 <- lm(log10(All.interactions + 1) ~ Paid + Category, data = facebook)
summary(fit3)</pre>
```

```
##
## Call:
## lm(formula = log10(All.interactions + 1) ~ Paid + Category, data = facebook)
##
## Residuals:
##
       Min
                1Q Median
                                30
                                        Max
## -1.95563 -0.23538 0.01645 0.26075 1.49121
##
## Coefficients:
##
                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                     1.80436 0.03615 49.907 < 2e-16 ***
## Paid
                     0.15127 0.04857 3.115 0.00195 **
## CategoryInspiration 0.39403 0.05121 7.695 7.74e-14 ***
## CategoryProduct
                     ## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.4859 on 495 degrees of freedom
    (1 observation deleted due to missingness)
## Multiple R-squared: 0.1433, Adjusted R-squared: 0.1382
## F-statistic: 27.61 on 3 and 495 DF, p-value: < 2.2e-16
Comments?
```

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Comments?

### Change response. A slightly different fitted model

```
fit4 <- lm(log10(All.interactions + 1) ~ Paid * Category, data = facebook)
summarv(fit4)
##
## Call:
## lm(formula = log10(All.interactions + 1) ~ Paid * Category, data = facebook)
##
## Residuals:
      Min
               10 Median
                              30
                                     Max
##
## -2.01793 -0.23100 0.02586 0.27246 1.51761
##
## Coefficients:
##
                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                        1.77795
                                 0.03941 45.111 < 2e-16 ***
## Paid
                        ## CategoryInspiration 0.46570 0.06040 7.711 6.96e-14 ***
## CategoryProduct
                     0.37776    0.06302    5.994    3.95e-09 ***
## Paid:CategoryProduct
                      -0.04374 0.12234 -0.358 0.72083
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.4843 on 493 degrees of freedom
    (1 observation deleted due to missingness)
## Multiple R-squared: 0.1524, Adjusted R-squared: 0.1438
## F-statistic: 17.72 on 5 and 493 DF, p-value: 3.639e-16
```



### Change response. A slightly different fitted model

fit4\$coefficients

```
##
                (Intercept)
                                                  Paid
                                                            CategoryInspiration
##
                 1.77795481
                                           0.23997989
                                                                     0.46569543
##
            CategoryProduct Paid:CategoryInspiration
                                                           Paid:CategoryProduct
##
                 0.37776394
                                          -0.25185230
                                                                     -0.04374152
head(model.matrix(fit4))
```

```
##
     (Intercept) Paid CategoryInspiration CategoryProduct Paid:CategoryInspiration
## 1
                                                                                      0
                     0
## 2
                                                                                      0
## 3
## 4
## 5
                                                                                      0
## 6
##
     Paid:CategoryProduct
## 1
## 2
                         0
## 3
                         0
## 4
## 5
## 6
                         0
```



### Change explanatory variates to two factors

```
fit5 <- lm(log10(All.interactions + 1) - Type * Category, data = facebook)
summary(fit5)</pre>
```

```
##
## Call:
## lm(formula = log10(All.interactions + 1) ~ Type * Category, data = facebook)
##
## Residuals:
                 1Q Median
       Min
                                         Max
## -1.83783 -0.23716 0.01508 0.25688 1.60199
##
## Coefficients: (2 not defined because of singularities)
                                Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                                 1.73278
                                           0.10895 15.904
                                                            <2e-16 ***
## TypePhoto
                                0.10504
                                           0.11469
                                                   0.916
                                                            0.3602
## TypeStatus
                                0.36213
                                           0.30167 1.200
                                                            0.2306
                                           0.21397 3.039
## TypeVideo
                               0.65020
                                                            0.0025 **
## CategoryInspiration
                               0.20172 0.49927 0.404
                                                            0.6864
## CategoryProduct
                                           0.49927
                                                    -0.068
                                                            0.9460
                                -0.03381
## TypePhoto:CategoryInspiration
                               0.20383
                                           0.50213
                                                    0.406
                                                            0.6850
## TypeStatus:CategoryInspiration -0.09280
                                           0.62270 -0.149
                                                            0.8816
## TypeVideo:CategoryInspiration
                                     NA
                                                NΑ
                                                       NA
                                                                NΑ
## TypePhoto:CategoryProduct
                               0.39575
                                           0.50315
                                                   0.787
                                                            0.4319
## TypeStatus:CategoryProduct
                                                            0.7764
                               0.16441
                                           0.57849
                                                     0.284
## TypeVideo:CategoryProduct
                                     NA
                                                NΑ
                                                       NA
                                                                NA
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.4872 on 490 degrees of freedom
## Multiple R-squared: 0.1473, Adjusted R-squared: 0.1316
## F-statistic: 9.405 on 9 and 490 DF, p-value: 3.024e-13
```



### Just the coefficients.

#### fit5\$coefficients

```
##
                       (Intercept)
                                                         TypePhoto
                        1.73278345
                                                        0.10504178
##
##
                        TypeStatus
                                                         TypeVideo
                        0.36213204
                                                         0.65020444
##
##
                                                   CategoryProduct
              CategoryInspiration
##
                        0.20171500
                                                       -0.03381344
##
    TypePhoto:CategoryInspiration TypeStatus:CategoryInspiration
##
                        0.20382942
                                                       -0.09279854
##
    TypeVideo: Category Inspiration
                                         TypePhoto:CategoryProduct
##
                                NA
                                                         0.39574802
##
       TypeStatus: CategoryProduct
                                         TypeVideo: CategoryProduct
##
                        0.16440892
                                                                 NΑ
```



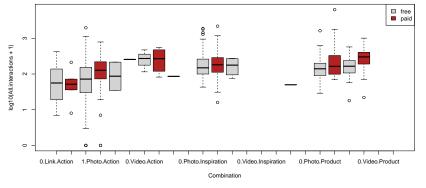
### And now the corresponding model matrix.

head(model.matrix(fit5))

```
(Intercept) TypePhoto TypeStatus TypeVideo CategoryInspiration
     CategoryProduct TypePhoto:CategoryInspiration TypeStatus:CategoryInspiration
## 2
## 6
     TypeVideo:CategoryInspiration TypePhoto:CategoryProduct
## 1
## 2
## 3
## 5
## 6
     TypeStatus:CategoryProduct TypeVideo:CategoryProduct
## 1
## 2
## 6
```

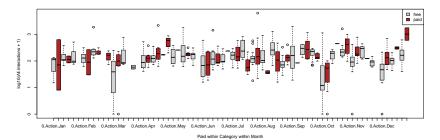


### Or how about?





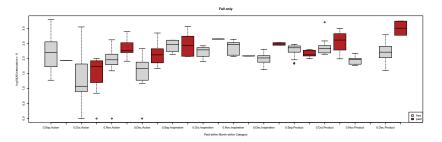
### 





### Focus only on Fall

```
Fall <- facebook$Post.Month %in% 9:12
with(facebook[Fall,], {
   boxplot(log10(All.interactions + 1) - Paid + cut(Post.Month, 4, labels = month.abb[9:12])+ Category ,
        xlab = "Paid within Month within Category", main = "Fall only",
        col = rep(c("lightgrey", "firebrick"), 4 * length(Category)))
   legend("bottomright", legend = c("free", "paid"), fill = c("lightgrey", "firebrick"))
}
</pre>
```

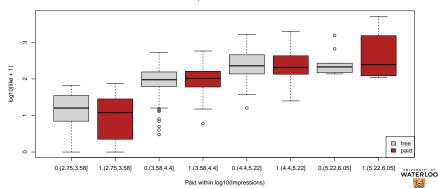




Could use cut() on the continuous (ratio-scaled) variate to turn it into a categorical and proceed as before.

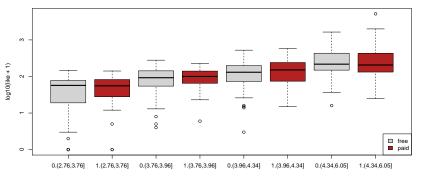
For example equal width intervals:

#### Equal width intervals



### Or perhaps four intervals of equal numbers

#### **Equal count intervals**



Paid within log10(Impressions)



Alternatively, we could build a (perhaps complicated) linear model, say modelling the mean of response Y as a polynomial of explanatory variate x:

$$\mu(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_p x^p$$

(or as any other linear (in the coefficients) model).



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$$\mu(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_p x^p$$

(or as any other linear (in the coefficients) model).

Such models can be fitted by least-squares.



Alternatively, we could build a (perhaps complicated) linear model, say modelling the mean of response Y as a polynomial of explanatory variate x:

$$\mu(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_p x^p$$

(or as any other linear (in the coefficients) model).

Such models can be fitted by least-squares.

Unfortunately, these models require a parametric form (e.g. a polynomial) be specified that will fit the data **everywhere** (i.e. globally for all x).

Alternatively, we could try fitting many simple functions of x locally, different at every value of x. Connecting the fitted values together produces an estimated  $\mu(x)$ 



For example, while we might not be willing to have one line fit all points, we might be willing to have *different lines* fitted in separate (and contiguous) regions of x.



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We can fit locally by using weighted least squares which minimizes

$$\sum_{i=1}^{n} w_{i}(x) (y_{i} - \mu(x_{i}))^{2}$$

where  $w_i(x)$  depends on the location x where we are fitting  $\mu(x)$ .



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We can fit locally by using weighted least squares which minimizes

$$\sum_{i=1}^{n} w_i(x) (y_i - \mu(x_i))^2$$

where  $w_i(x)$  depends on the location x where we are fitting  $\mu(x)$ . We fit  $\mu(x)$  for every x on in the range of the data.



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where  $w_i(x)$  depends on the location x where we are fitting  $\mu(x)$ . We fit  $\mu(x)$  for every x on in the range of the data.

We could also make the weight function  $w_i(x)$  to be 1 for those  $x_i$  near x and 0 for those far away. In this way, the weights determine the  $x_i$  values that contribute to fitting  $\mu(x)$  and those which do not.



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For example, for the *i*th observation  $x_i$  when fitting at any point x we could have

$$w_i(x) = K\left(\frac{x_i - x}{a}\right)$$

for some a>0 and function  $K(t)\geq 0$  that is maximal at (t=0) and decreasing with |t|.



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We can fit locally by using weighted least squares which minimizes

$$\sum_{i=1}^{n} w_{i}(x) (y_{i} - \mu(x_{i}))^{2}$$

where  $w_i(x)$  depends on the location x where we are fitting  $\mu(x)$ . We fit  $\mu(x)$  for every x on in the range of the data.

We could also make the weight function  $w_i(x)$  to be 1 for those  $x_i$  near x and 0 for those far away. In this way, the weights determine the  $x_i$  values that contribute to fitting  $\mu(x)$  and those which do not.

For example, for the *i*th observation  $x_i$  when fitting at any point x we could have

$$w_i(x) = K\left(\frac{x_i - x}{a}\right)$$

for some a>0 and function  $K(t)\geq 0$  that is maximal at (t=0) and decreasing with |t|.

The constant a controls the size of the region (i.e. which  $x_i$ s) that will be use to fit at x.

For example, while we might not be willing to have one line fit all points, we might be willing to have *different lines* fitted in separate (and contiguous) regions of x. That is we could fit lines **locally** within each region of x.

We can fit locally by using weighted least squares which minimizes

$$\sum_{i=1}^{n} w_{i}(x) (y_{i} - \mu(x_{i}))^{2}$$

where  $w_i(x)$  depends on the location x where we are fitting  $\mu(x)$ . We fit  $\mu(x)$  for every x on in the range of the data.

We could also make the weight function  $w_i(x)$  to be 1 for those  $x_i$  near x and 0 for those far away. In this way, the weights determine the  $x_i$  values that contribute to fitting  $\mu(x)$  and those which do not.

For example, for the *i*th observation  $x_i$  when fitting at any point x we could have

$$w_i(x) = K\left(\frac{x_i - x}{a}\right)$$

for some a>0 and function  $K(t)\geq 0$  that is maximal at (t=0) and decreasing with |t|.

The constant a controls the size of the region (i.e. which  $x_i$ s) that will be used to fit at x. The smaller these regions were, the less structure we would be imposing on the underlying function  $\mu(x)$ .

In R there is a function called loess that fits a locally weighted sum of squares estimate that pays a little more attention to some of these problems.

```
loess(formula, data, ..., span = 0.75, ...)
```

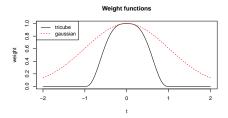


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As its default weight function loess uses Tukey's tri-cube weight

$$\mathcal{K}(t) = \left\{ egin{array}{ll} (1-|t|^3)^3 & t \in [-1,1] \ 0 & ext{otherwise}. \end{array} 
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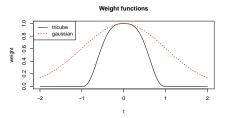




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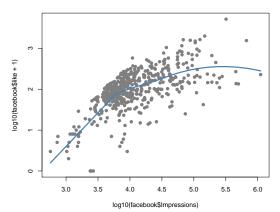


This is generally more resistant to outlying  $x_i$ s than, say, a Gaussian weight function (i.e.  $K(W) = \phi(w)$  the N(0,1) density).

N.B. loess is not restricted to fitting local lines. It can fit any degree polynomial locally (though typically only degree 1 or 2 is used in practice).



#### Loess smooth





#### Loess smooth

